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# Simulation of ozonolysis reactions by the master equation approach and adaption of the code for use on a supercomputer

Najoua Derbel<sup>1,2</sup>, Alexander Alijah<sup>\*3</sup>, Struan H Robertson<sup>4</sup>, Lilian Joly<sup>3</sup>, Thomas Lauvaux<sup>3</sup>, and Patrick Bousquet-Melou<sup>\*5</sup>

<sup>1</sup>Laboratoire de Spectroscopie Atomique, Moléculaire et Applications – Tunisie

<sup>2</sup>Faculté des Sciences de Bizerte [Université de Carthage] – Tunisie

<sup>3</sup>Groupe de spectrométrie moléculaire et atmosphérique – Université de Reims Champagne-Ardenne : UMR7331, Centre National de la Recherche Scientifique : UMR7331, Université de Reims Champagne-Ardenne, Centre National de la Recherche Scientifique – France

<sup>4</sup>Dassault-Systèmes – Royaume-Uni

<sup>5</sup>Centre Régional Informatique et d'Applications Numériques de Normandie (CRIANN) – CRIANN – France

## Résumé

### Scientific problem:

Plants in a situation of stress caused by polluted environments emit chemical compounds known as terpenes, which are then decomposed by molecules present in smog such as ozone. Our aim is to identify the decomposition products as these may serve as biomarkers for oxidative stress.

### Scientific algorithm:

The reaction mechanism of ozonolysis is highly complex (1, 2), and the resulting coupled differential equations are difficult to solve by conventional methods. We therefore used the free master equation solver MESMER developed by Robertson and colleagues (3) which treats chemical reactions as collisional energy transfers. It is capable of solving the energy grained master equation for a unimolecular system composed of an arbitrary number of wells, transition states, sinks, and reactants.

### Difficulties to overcome:

However it requires a very long CPU time, up to several days, for our reaction system, and sometimes it even fails because of the stiffness of the differential equations. Furthermore, the code was not meant to be applied to such a complex system and is not adapted to parallel execution, except for the embarrassingly parallel mode if solutions at several temperatures are sought.

### Solution:

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\*Intervenant

We tried to solve the problem with the following approach:

- 1) Identify the chemical reactions that are extremely slow and may be omitted such as to reduce the size of the system of coupled equations and to reduce the stiffness
- 2) Transfer the code to the NEC-SX Aurora TSUBASA vector computer at CRIANN. Code profiling showed overly structured C++ programming, inhibiting vectorization, so that the specialized Aurora architecture and the code are too poorly adapted to each other.
- 3) Adapt the computer code for use on parallel supercomputers of more standard architecture, such as Austral at CRIANN. In the most computationally demanding matrix diagonalization function, the innermost loop can be parallelized by OpenMP threads.
- 4) Choose advanced compilation options and enhanced runtime options: as the code is identified as compute-bound, enabling turbo boost (at user job level) on AMD Genoa processors is effective.

Results :

A speedup of more than 4.

The lightning talk and poster will present the scientific objectives and results. They will also describe the computational performance gains achieved through improved models and HPC programming and execution techniques.

References:

- (1) N. Derbel, C. Kalalian, A. Alijah, S. H. Robertson, A. Chakir and E. Roth, "Ozonolysis of 2-Methyl-2-pentenal: New Insights from Master Equation Modeling". *J. Phys. Chem. A* **128**, 2534-2542 (2025), DOI: 10.1021/acs.jpca.3c04965
- (2) N. Derbel, A. Alijah, S. H. Robertson, T. Lauvaux and L. Joly, "First-Generation Products of *Trans*-2-Hexenal Ozonolysis: A New Look at the Mechanism". *J. Phys. Chem. A* **129**, 3272-3279 (2025), DOI: 10.1021/acs.jpca.4c07608
- (3) D. R. Glowacki, C.-H. Liang, C. Morley, M. J. Pilling and S. H. Robertson, "MES-MER: An Open-Source Master Equation Solver for Multi-Energy Well Reactions". *J. Phys. Chem. A* **116**, 9545-9560 (2012), DOI: 10.1021/jp3051033